



wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 11:18 AM UTC

PDB ID : 8Y2H / pdb_00008y2h
EMDB ID : EMD-38855
Title : GK tetramer of AtP5CS1 filament with adjacent hooks, reaction state
Authors : Zhang, T.; Guo, C.J.; Liu, J.L.
Deposited on : 2024-01-26
Resolution : 3.30 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

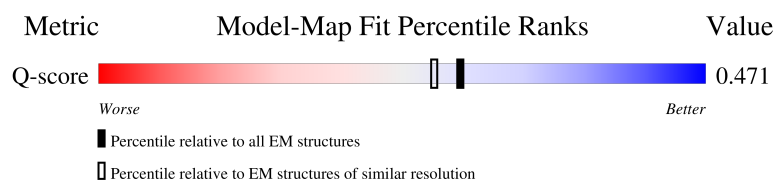
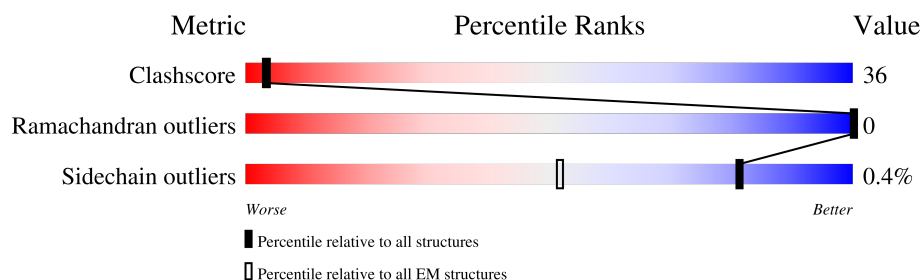
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15087 (2.80 - 3.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	727	98%
1	B	727	22% 14% 63%
1	C	727	98%
1	D	727	98%

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Mol	Chain	Length	Quality of chain
1	E	727	98%
1	F	727	22% 14% 63%
1	G	727	23% 14% 63%
1	H	727	22% 14% 63%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8808 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Delta-1-pyrroline-5-carboxylate synthase A.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	267	Total 2047	C 1289	N 361	O 391	S 6	0	0
1	A	15	Total 124	C 79	N 22	O 23		0	0
1	F	267	Total 2047	C 1289	N 361	O 391	S 6	0	0
1	C	15	Total 124	C 79	N 22	O 23		0	0
1	G	267	Total 2047	C 1289	N 361	O 391	S 6	0	0
1	D	15	Total 124	C 79	N 22	O 23		0	0
1	H	267	Total 2047	C 1289	N 361	O 391	S 6	0	0
1	E	15	Total 124	C 79	N 22	O 23		0	0

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-9	MET	-	initiating methionine	UNP P54887
B	-8	GLY	-	expression tag	UNP P54887
B	-7	SER	-	expression tag	UNP P54887
B	-6	SER	-	expression tag	UNP P54887
B	-5	HIS	-	expression tag	UNP P54887
B	-4	HIS	-	expression tag	UNP P54887
B	-3	HIS	-	expression tag	UNP P54887
B	-2	HIS	-	expression tag	UNP P54887
B	-1	HIS	-	expression tag	UNP P54887
B	0	HIS	-	expression tag	UNP P54887
A	-9	MET	-	initiating methionine	UNP P54887
A	-8	GLY	-	expression tag	UNP P54887
A	-7	SER	-	expression tag	UNP P54887
A	-6	SER	-	expression tag	UNP P54887

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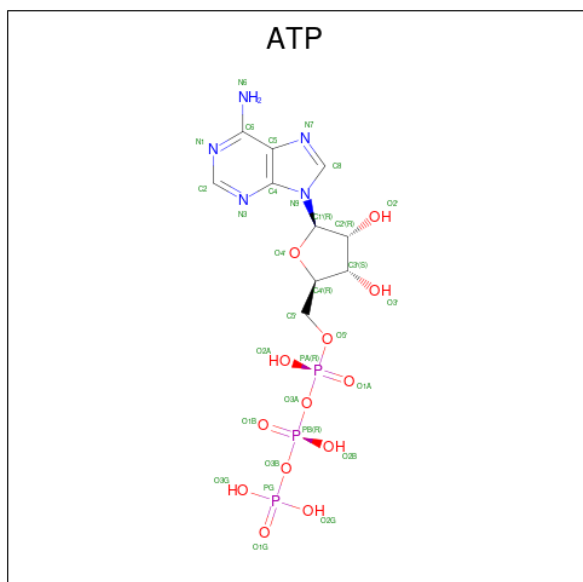
Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	HIS	-	expression tag	UNP P54887
A	-4	HIS	-	expression tag	UNP P54887
A	-3	HIS	-	expression tag	UNP P54887
A	-2	HIS	-	expression tag	UNP P54887
A	-1	HIS	-	expression tag	UNP P54887
A	0	HIS	-	expression tag	UNP P54887
F	-9	MET	-	initiating methionine	UNP P54887
F	-8	GLY	-	expression tag	UNP P54887
F	-7	SER	-	expression tag	UNP P54887
F	-6	SER	-	expression tag	UNP P54887
F	-5	HIS	-	expression tag	UNP P54887
F	-4	HIS	-	expression tag	UNP P54887
F	-3	HIS	-	expression tag	UNP P54887
F	-2	HIS	-	expression tag	UNP P54887
F	-1	HIS	-	expression tag	UNP P54887
F	0	HIS	-	expression tag	UNP P54887
C	-9	MET	-	initiating methionine	UNP P54887
C	-8	GLY	-	expression tag	UNP P54887
C	-7	SER	-	expression tag	UNP P54887
C	-6	SER	-	expression tag	UNP P54887
C	-5	HIS	-	expression tag	UNP P54887
C	-4	HIS	-	expression tag	UNP P54887
C	-3	HIS	-	expression tag	UNP P54887
C	-2	HIS	-	expression tag	UNP P54887
C	-1	HIS	-	expression tag	UNP P54887
C	0	HIS	-	expression tag	UNP P54887
G	-9	MET	-	initiating methionine	UNP P54887
G	-8	GLY	-	expression tag	UNP P54887
G	-7	SER	-	expression tag	UNP P54887
G	-6	SER	-	expression tag	UNP P54887
G	-5	HIS	-	expression tag	UNP P54887
G	-4	HIS	-	expression tag	UNP P54887
G	-3	HIS	-	expression tag	UNP P54887
G	-2	HIS	-	expression tag	UNP P54887
G	-1	HIS	-	expression tag	UNP P54887
G	0	HIS	-	expression tag	UNP P54887
D	-9	MET	-	initiating methionine	UNP P54887
D	-8	GLY	-	expression tag	UNP P54887
D	-7	SER	-	expression tag	UNP P54887
D	-6	SER	-	expression tag	UNP P54887
D	-5	HIS	-	expression tag	UNP P54887
D	-4	HIS	-	expression tag	UNP P54887

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-3	HIS	-	expression tag	UNP P54887
D	-2	HIS	-	expression tag	UNP P54887
D	-1	HIS	-	expression tag	UNP P54887
D	0	HIS	-	expression tag	UNP P54887
H	-9	MET	-	initiating methionine	UNP P54887
H	-8	GLY	-	expression tag	UNP P54887
H	-7	SER	-	expression tag	UNP P54887
H	-6	SER	-	expression tag	UNP P54887
H	-5	HIS	-	expression tag	UNP P54887
H	-4	HIS	-	expression tag	UNP P54887
H	-3	HIS	-	expression tag	UNP P54887
H	-2	HIS	-	expression tag	UNP P54887
H	-1	HIS	-	expression tag	UNP P54887
H	0	HIS	-	expression tag	UNP P54887
E	-9	MET	-	initiating methionine	UNP P54887
E	-8	GLY	-	expression tag	UNP P54887
E	-7	SER	-	expression tag	UNP P54887
E	-6	SER	-	expression tag	UNP P54887
E	-5	HIS	-	expression tag	UNP P54887
E	-4	HIS	-	expression tag	UNP P54887
E	-3	HIS	-	expression tag	UNP P54887
E	-2	HIS	-	expression tag	UNP P54887
E	-1	HIS	-	expression tag	UNP P54887
E	0	HIS	-	expression tag	UNP P54887

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).

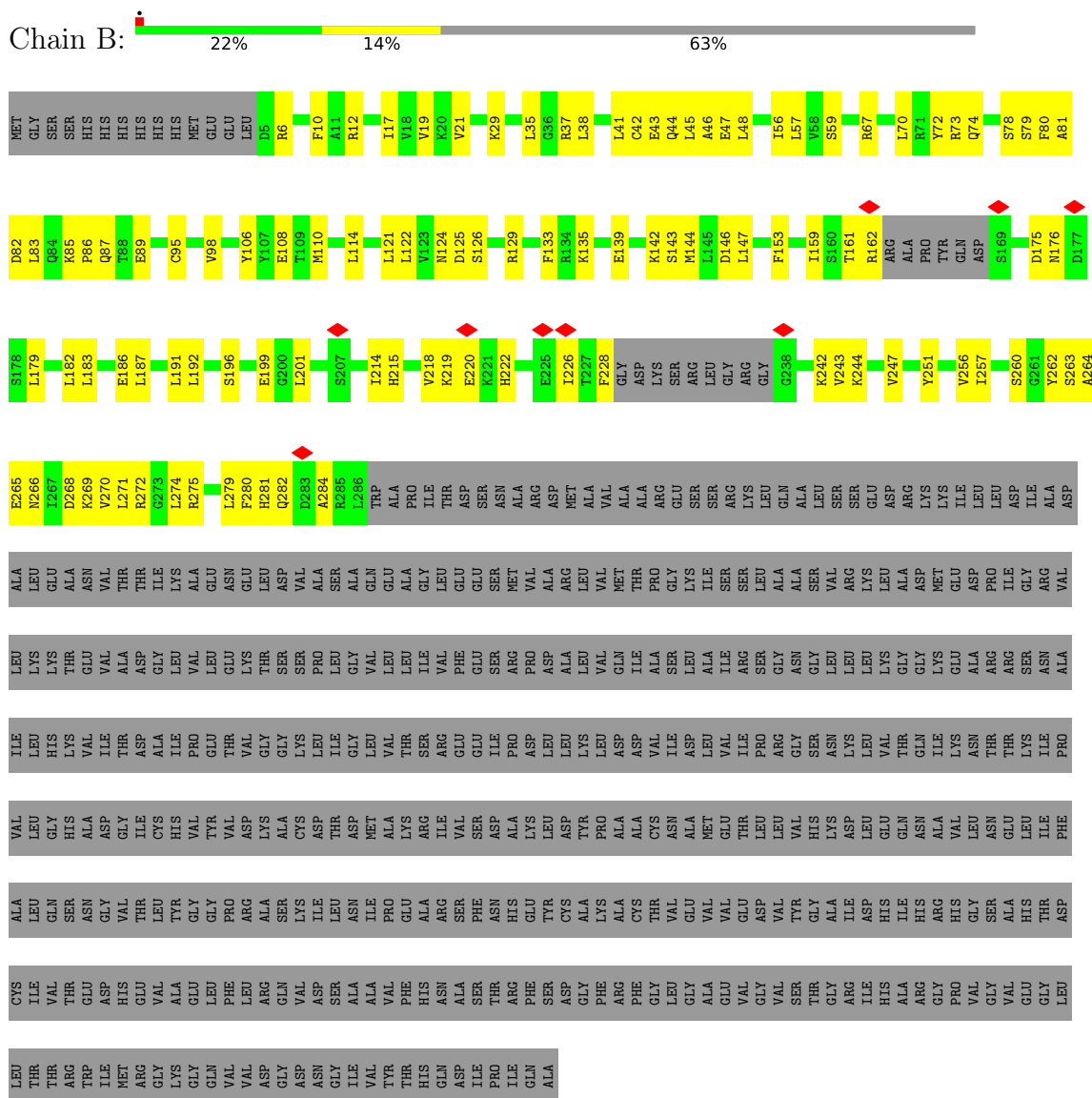


Mol	Chain	Residues	Atoms					AltConf
2	B	1	Total 31	C 10	N 5	O 13	P 3	0
2	F	1	Total 31	C 10	N 5	O 13	P 3	0
2	G	1	Total 31	C 10	N 5	O 13	P 3	0
2	H	1	Total 31	C 10	N 5	O 13	P 3	0

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Delta-1-pyrroline-5-carboxylate synthase A



• Molecule 1: Delta-1-pyrroline-5-carboxylate synthase A

98%



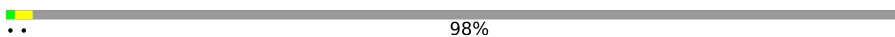
63%



ARG	THR	SER	HIS	LYS	THR	ALA	D268
THR	GLU	ASN	ALA	VAL	GLU	ASN	D269
ILE	ASP	GLY	ASP	ILE	VAL	VAL	V270
MET	HIS	VAL	GLY	THR	ALA	THR	L271
GLY	VAL	THR	ILE	ASP	ASP	THR	R272
LYS	ALA	LEU	CYS	ALA	GLY	ILE	G273
GLY	GLU	TYR	HIS	ILE	LEU	LYS	L274
GLN	LEU	GLY	VAL	PRO	VAL	ALA	R275
VAL	PHE	PRO	VAL	THR	GLU	GLU	L279
VAL	LEU	ARG	ASP	VAL	LYS	GLU	F280
ASP	ARG	ALA	LYS	GLY	THR	LEU	H281
GLY	GLN	SER	ALA	GLY	SER	ASP	Q282
ASN	VAL	ILE	CYS	LYS	SER	VAL	D283
ASN	ASP	ILE	ASP	LEU	PRO	ALA	A284
GLY	SER	LEU	THR	ILE	LEU	SER	F285
ILE	ALA	ASN	ASP	GLY	GLY	ALA	L286
VAL	VAL	ILE	MET	LEU	VAL	GLN	THR
TYR	VAL	PRO	ALA	VAL	LEU	GLU	ALA
PHE	PHE	GLU	LYS	THR	ALA	PRO	PRO
HIS	HIS	ALA	ARG	SER	ILE	GLY	ILE
GLN	ASN	ARG	ILE	ARG	VAL	THR	THR
ASP	ALA	SER	VAL	GLU	PHE	GLU	ASP
ILE	SER	PHE	SER	GLU	GLU	ASP	SER
PRO	THR	ASN	ASP	ILE	SER	ASN	ASN
ILE	PHE	HIS	ALA	PRO	ARG	MET	ALA
GLN	ARG	GLU	LYS	ASP	VAL	VAL	ARG
ALA	SER	TYR	LEU	LEU	ALA	ARG	ASP
	GLY	CYS	ASP	LEU	ARG	ALA	MET
	GLY	ALA	TYR	LYS	LEU	LEU	ALA
	PHE	ALA	PRO	LEU	VAL	VAL	VAL
	ARG	ALA	ALA	ASP	GLN	MET	ALA
	GLY	CYS	ALA	ASP	THR	THR	ALA
	GLY	THR	CYS	VAL	ALA	PRO	ALA
	LEU	VAL	ASN	ILE	SER	GLY	ARG
	GLY	GLU	ALA	ASP	LEU	LYS	GLU
	ALA	VAL	MET	ILE	ALA	ILE	SER
	GLU	VAL	GLU	LEU	ALA	ILE	SER
	VAL	GLU	THR	ILE	ARG	SER	ARG
	GLY	ASP	GLU	PRO	SER	LEU	LEU
	VAL	VAL	LEU	ARG	GLY	ALA	GLN
	SER	TYR	VAL	GLY	ASN	ALA	ALA
	THR	GLY	HIS	SER	GLY	SER	LEU
	GLY	ALA	LYS	ASN	VAL	VAL	SER
	ARG	ILE	ASP	LYS	ARG	LYS	GLU
	ILE	ASP	LEU	LEU	LYS	LEU	ASP
	HIS	HIS	GLU	VAL	THR	ALA	ARG
	ALA	ILE	GLN	THR	GLY	LYS	LYS
	ARG	HIS	ASN	GLN	GLY	ASP	ARG
	GLY	ARG	ALA	ILE	LYS	MET	THR
	PRO	HIS	VAL	LYS	GLU	GLU	ILE
	VAL	GLY	LEU	ASN	ALA	ASP	LEU
	GLY	SER	ASN	THR	ARG	PRO	LEU
	VAL	ALA	GLU	THR	ARG	ILE	ASP
	GLU	HIS	LEU	LYS	GLY	GLY	ASP
	GLY	THR	ILE	ILE	SER	THR	ILE
	LEU	ASP	PHE	PRO	ILE	VAL	ALA
	LEU	CYS	ALA	VAL	ILE	LEU	ASP
	THR	VAL	GLN	LYS	THR	LYS	LEU

- Molecule 1: Delta-1-pyrroline-5-carboxylate synthase A

Chain C:  ..

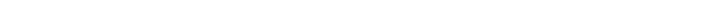


98%

[illegible]

[illegible]

- Molecule 1: Delta-1-pyrroline-5-carboxylate synthase A

Chain H:  22% 14% 63%

ALA	D268	S178	K85	MET
ASN	K269	L179	P86	GLY
VAL	V270	L182	Q87	SER
THR	L271	L182	T88	SER
THR	R272	E186	E89	HIS
ILE	G273	L187	K93	HIS
LYS	L274	L191	A94	HIS
ALA	R275	L192	C95	HIS
GLU		S196	V98	MET
GLU	L279	E199	M104	GLU
F280	D283	A105	A105	GLU
H281	A284	A106	V107	LEU
ASP	Q282	S207	E108	D5
VAL	D283		T109	R6
ALA	A284	H215	M110	F10
SER	R285	V218	L114	A11
SER	L286	E220	Q120	R12
GLN	TRP	K221	L121	I17
GLU	ALA	H222	L122	V18
ALA	ALA	Q223	D125	V19
ALA	ALA	D224	R129	K20
GLU	ASP	E225	F133	V21
ALA	ASP	F228	R134	K29
ALA	MET	GLY	K135	R37
GLY	LEU	ASP	E139	L38
ILE	ILE	LYS	T140	L41
GLU	VAL	SER	E141	C42
THR	ALA	ARG	GLY	E43
PRO	ALA	LEU	ARG	Q44
THR	ALA	ILE	K142	L45
ASP	ALA	SER	S143	A46
GLY	VAL	ARG	D146	E47
GLU	VAL	LYS	L147	S56
LEU	LEU	LEU	F153	S57
ALA	ALA	GLN	I159	R67
ALA	ALA	ASP	S160	Q68
SER	LEU	ARG	T161	R69
VAL	SER	LYS	R162	L70
VAL	SER	ILE	ARG	R73
ARG	SER	T254	ALA	Q74
LYS	GLU	P255	PRO	S78
LEU	ASP	V256	TYR	S79
LEU	ASP	Y251	GLN	F90
ALA	ASP	I	ASP	A81
ALA	ALA	K242	S169	D82
VAL	ALA	V243	D175	L83
VAL	ALA	K244	N176	K84
ARG	LEU	ILE	D177	
LYS	LEU	LYS		
LEU	LEU	LEU		
LEU	ASP	ASP		
ILE	ILE	ILE		
ARG	ARG	VAL		
VAL	VAL	LEU		
LYS	LYS	LEU		
LYS	LYS	GLU		

ARG	THR	SER	HIS	LYS	THR
TRP	ASP	ASN	ASP	VAL	THR
ILE	ASP	GLY	ALA	ILE	VAL
MET	HIS	VAL	GLY	THR	ASP
ARG	GLU	THR	ILE	ASP	ALA
GLY	VAL	LEU	CYS	ILE	GLY
LYS	ALA	TYR	HIS	ILE	LEU
GLY	GLU	GLY	VAL	PRO	VAL
GLN	LEU	GLY	TYR	THR	GLU
VAL	PHE	PRO	VAL	THR	GLU
ASP	LEU	ARG	ASP	VAL	LYS
VAL	ARG	ALA	LYS	GLY	THR
GLY	GLN	SER	ALA	GLY	THR
ASP	VAL	SER	ILE	LEU	VAL
GLY	GLN	SER	ALA	LEU	LEU
ASP	VAL	ASN	MET	VAL	VAL
GLY	THR	PRO	ALA	VAL	LEU
ASP	PHE	GLU	LYS	THR	LEU
ASN	HIS	ALA	ARG	SER	ILE
GLY	ASN	ARG	ILE	ARG	THR
ILE	GLN	ARG	ILE	ARG	THR
ASP	ASP	SER	VAL	GLU	PHE
ILE	SER	PHE	SER	GLU	GLY
PRO	THR	ASN	ASP	ILE	SER
ILE	ARG	HIS	ALA	PRO	ARG
GLN	PHE	GLU	ALA	ASP	PRO
ALA	ASP	TYR	LEU	LEU	ASP
	ASP	CYS	ASP	LEU	ALA
	GLY	ALA	TYR	LYS	LEU
	PHE	LYS	PRO	LEU	VAL
	ARG	ALA	ALA	ASP	GLN
	PHE	CYS	ALA	ASP	ILE
	GLY	THR	CYS	VAL	ALA
	LEU	VAL	ASN	ILE	SER
	GLY	GLU	ALA	ASP	LEU
	ALA	VAL	MET	LEU	LEU
	GLU	VAL	GLU	VAL	VAL
	VAL	GLU	THR	ILE	ARG
	GLY	ASP	LEU	PRO	GLY
	VAL	VAL	LEU	ARG	GLY
	SER	TYR	VAL	GLY	ASN
	THR	GLY	HIS	SER	GLY
	GLY	ALA	LYS	ASN	LEU
	ARG	ILE	ASP	LYS	LEU
	ILE	ASP	LEU	LEU	LEU
	HIS	HIS	GLU	VAL	LYS
	ALA	ILE	GLN	THR	GLY
	ARG	HIS	ASN	GLY	GLY
	GLY	ARG	ALA	ILE	LYS
	PRO	HIS	VAL	LYS	GLU
	VAL	GLY	LEU	ASN	ALA
	GLY	SER	ASN	THR	ARG
	VAL	ALA	GLU	THR	ARG
	GLY	HIS	LEU	LYS	SER
	GLY	THR	ILE	ILE	ASN
	LEU	ASP	PHE	PRO	ALA
	LEU	CYS	ALA	VAL	ILE
	THR	ILE	LEU	LEU	THR
	THR	VAL	GLN	GLY	HIS

- Molecule 1: Delta-1-pyrroline-5-carboxylate synthase A

Chain E: 98%

ASP	ILE	PRO	ILE	GLN	ALA	SER	VAL	GLU	PHE	GLU	GLU	ASP	SER	SER	ARG	ILE	ASP	ILE	ASP	GLW	ASP	ASP	GLY	MET
ILE	SER	THR	THR	ARG	THR	PHE	ASP	ILE	SER	GLU	GLU	ASN	SER	ASN	LEU	THR	LEU	THR	LEU	THR	GLW	GLY	GLY	SER
ILE	ARG	PHE	ILE	GLN	THR	GLU	LYS	ASP	PRO	ARG	VAL	ALA	PRO	ALA	GLY	ARG	ASP	GLY	ASP	ASP	VAL	GLU	GLY	SER
SER	THR	SER	THR	SER	THR	THR	LEU	LEU	ASP	ASP	ALA	ALA	ASP	ASP	GLY	GLY	THR	THR	THR	THR	THR	ILE	THR	HIS
ASP	GLY	THR	THR	THR	THR	THR	CYS	ASP	CYS	ALA	VAL	VAL	THR	ALA	ARG	VAL	LEU	LEU	ALA	ALA	VAL	LEU	LEU	HIS
GLY	THR	THR	THR	THR	THR	THR	VAL	ILE	SER	ALA	PRO	GLY	GLU	GLU	VAL	LYS	VAL	VAL	VAL	VAL	VAL	VAL	VAL	HIS
THR	THR	THR	THR	THR	THR	THR	ASP	ASP	THR	GLU	GLU	ILE	ASP	ASP	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	HIS
PHE	THR	THR	THR	THR	THR	THR	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	HIS
GLY	THR	THR	THR	THR	THR	THR	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	HIS
THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	HIS
THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	HIS
THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	HIS
THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	HIS
THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	HIS
THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	HIS
THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	HIS
THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	HIS
THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	HIS
THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	HIS
THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	HIS
THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	HIS
THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	HIS
THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	HIS
THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	HIS
THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	HIS
THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	HIS
THR	THR	THR	THR																					

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, D2	Depositor
Number of particles used	222855	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.2	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	3.470	Depositor
Minimum map value	-1.623	Depositor
Average map value	0.019	Depositor
Map value standard deviation	0.097	Depositor
Recommended contour level	0.5	Depositor
Map size ($\text{\AA}$)	254.4, 254.4, 254.4	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.06, 1.06, 1.06	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ATP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.87	0/126	1.10	0/169
1	B	0.43	0/2072	0.54	0/2794
1	C	0.87	0/126	1.09	0/169
1	D	0.87	0/126	1.09	0/169
1	E	0.88	0/126	1.10	0/169
1	F	0.43	0/2072	0.53	0/2794
1	G	0.44	0/2072	0.54	0/2794
1	H	0.44	0/2072	0.54	0/2794
All	All	0.47	0/8792	0.58	0/11852

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	124	0	122	20	0
1	B	2047	0	2084	147	0
1	C	124	0	122	23	0
1	D	124	0	122	22	0
1	E	124	0	122	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	2047	0	2084	149	0
1	G	2047	0	2084	150	0
1	H	2047	0	2084	142	0
2	B	31	0	12	0	0
2	F	31	0	12	0	0
2	G	31	0	12	0	0
2	H	31	0	12	0	0
All	All	8808	0	8872	637	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 36.

The worst 5 of 637 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:129:ARG:NH1	1:H:129:ARG:HA	1.58	1.18
1:F:129:ARG:HA	1:F:129:ARG:NH1	1.58	1.18
1:B:129:ARG:NH1	1:B:129:ARG:HA	1.58	1.18
1:G:129:ARG:HA	1:G:129:ARG:NH1	1.58	1.17
1:B:17:ILE:HD11	1:B:271:LEU:HD21	1.19	1.13

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	13/727 (2%)	11 (85%)	2 (15%)	0	100	100
1	B	261/727 (36%)	251 (96%)	10 (4%)	0	100	100
1	C	13/727 (2%)	11 (85%)	2 (15%)	0	100	100
1	D	13/727 (2%)	11 (85%)	2 (15%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	13/727 (2%)	11 (85%)	2 (15%)	0	100	100
1	F	261/727 (36%)	250 (96%)	11 (4%)	0	100	100
1	G	261/727 (36%)	250 (96%)	11 (4%)	0	100	100
1	H	261/727 (36%)	251 (96%)	10 (4%)	0	100	100
All	All	1096/5816 (19%)	1046 (95%)	50 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	14/597 (2%)	14 (100%)	0	100	100
1	B	220/597 (37%)	219 (100%)	1 (0%)	81	83
1	C	14/597 (2%)	14 (100%)	0	100	100
1	D	14/597 (2%)	14 (100%)	0	100	100
1	E	14/597 (2%)	14 (100%)	0	100	100
1	F	220/597 (37%)	218 (99%)	2 (1%)	70	78
1	G	220/597 (37%)	219 (100%)	1 (0%)	81	83
1	H	220/597 (37%)	220 (100%)	0	100	100
All	All	936/4776 (20%)	932 (100%)	4 (0%)	81	84

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	73	ARG
1	F	159	ILE
1	F	177	ASP
1	G	159	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such

sidechains are listed below:

Mol	Chain	Res	Type
1	G	222	HIS
1	H	282	GLN
1	E	84	GLN
1	F	124	ASN
1	B	124	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	ATP	H	801	-	32,33,33	0.30	0	48,52,52	0.41	0
2	ATP	F	801	-	32,33,33	0.30	0	48,52,52	0.41	0
2	ATP	B	801	-	32,33,33	0.30	0	48,52,52	0.41	0
2	ATP	G	801	-	32,33,33	0.30	0	48,52,52	0.41	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ATP	H	801	-	-	7/22/38/38	0/3/3/3
2	ATP	F	801	-	-	7/22/38/38	0/3/3/3
2	ATP	B	801	-	-	7/22/38/38	0/3/3/3
2	ATP	G	801	-	-	7/22/38/38	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

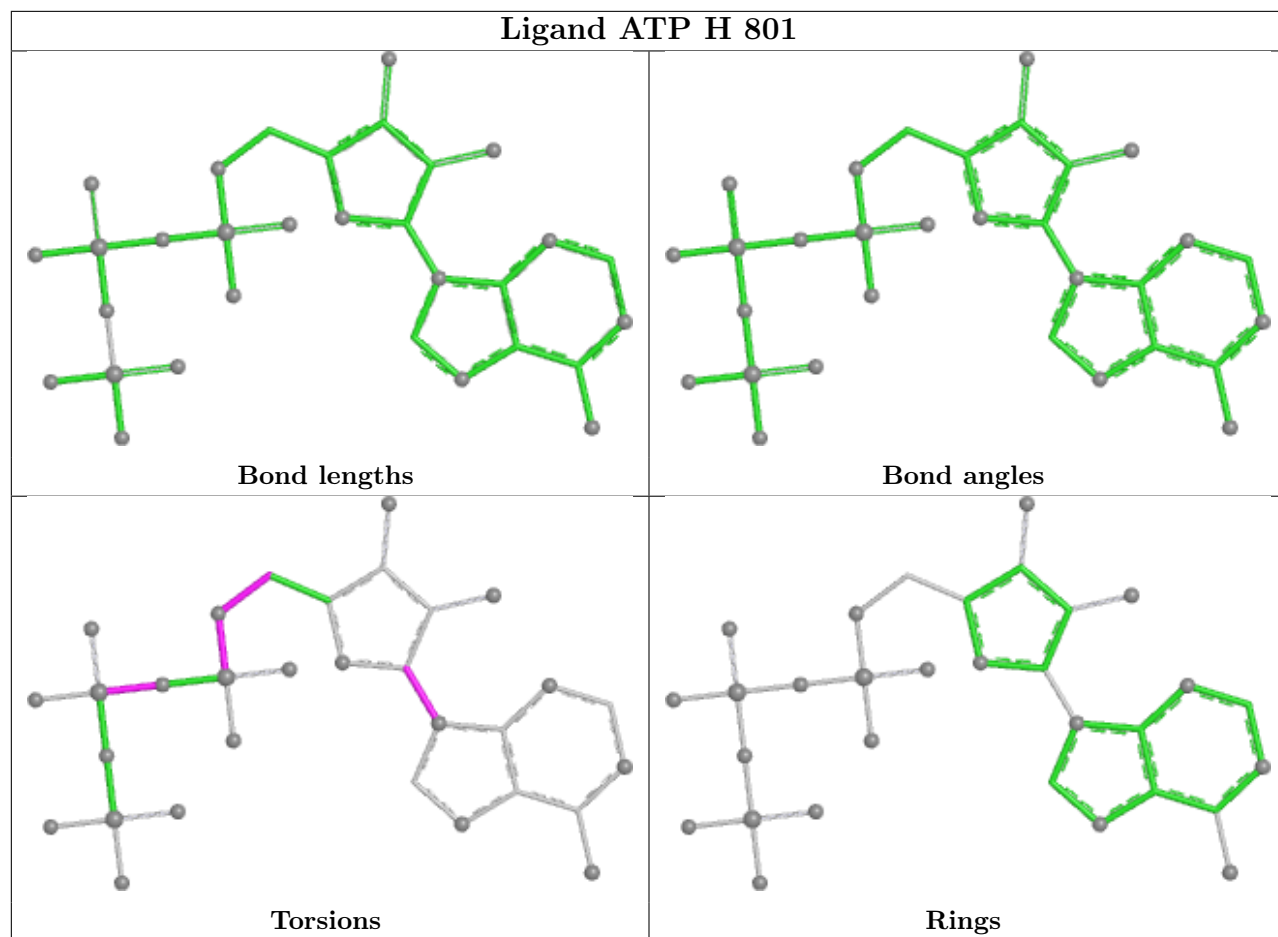
5 of 28 torsion outliers are listed below:

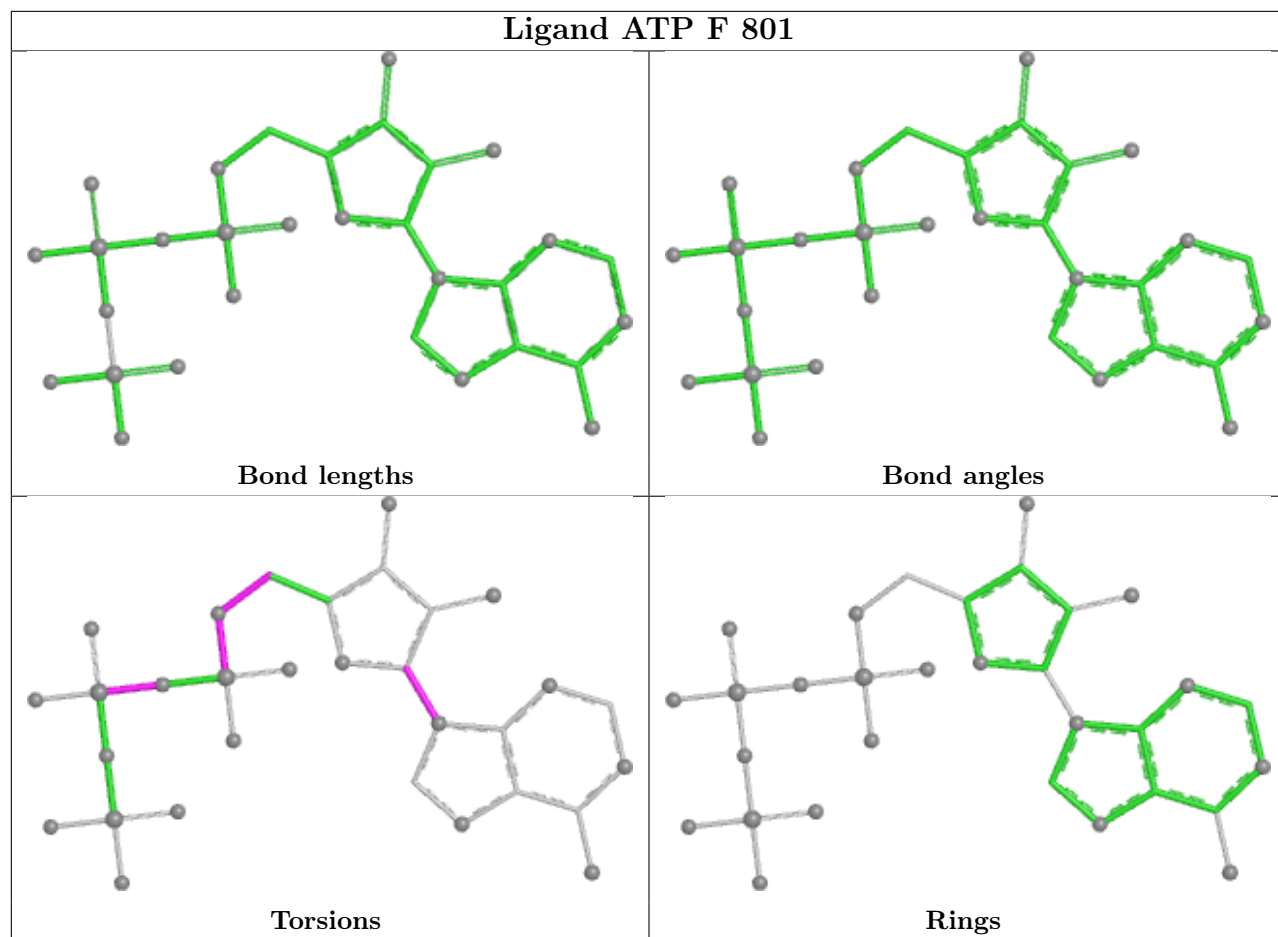
Mol	Chain	Res	Type	Atoms
2	B	801	ATP	C5'-O5'-PA-O1A
2	B	801	ATP	C5'-O5'-PA-O2A
2	B	801	ATP	C5'-O5'-PA-O3A
2	F	801	ATP	C5'-O5'-PA-O1A
2	F	801	ATP	C5'-O5'-PA-O2A

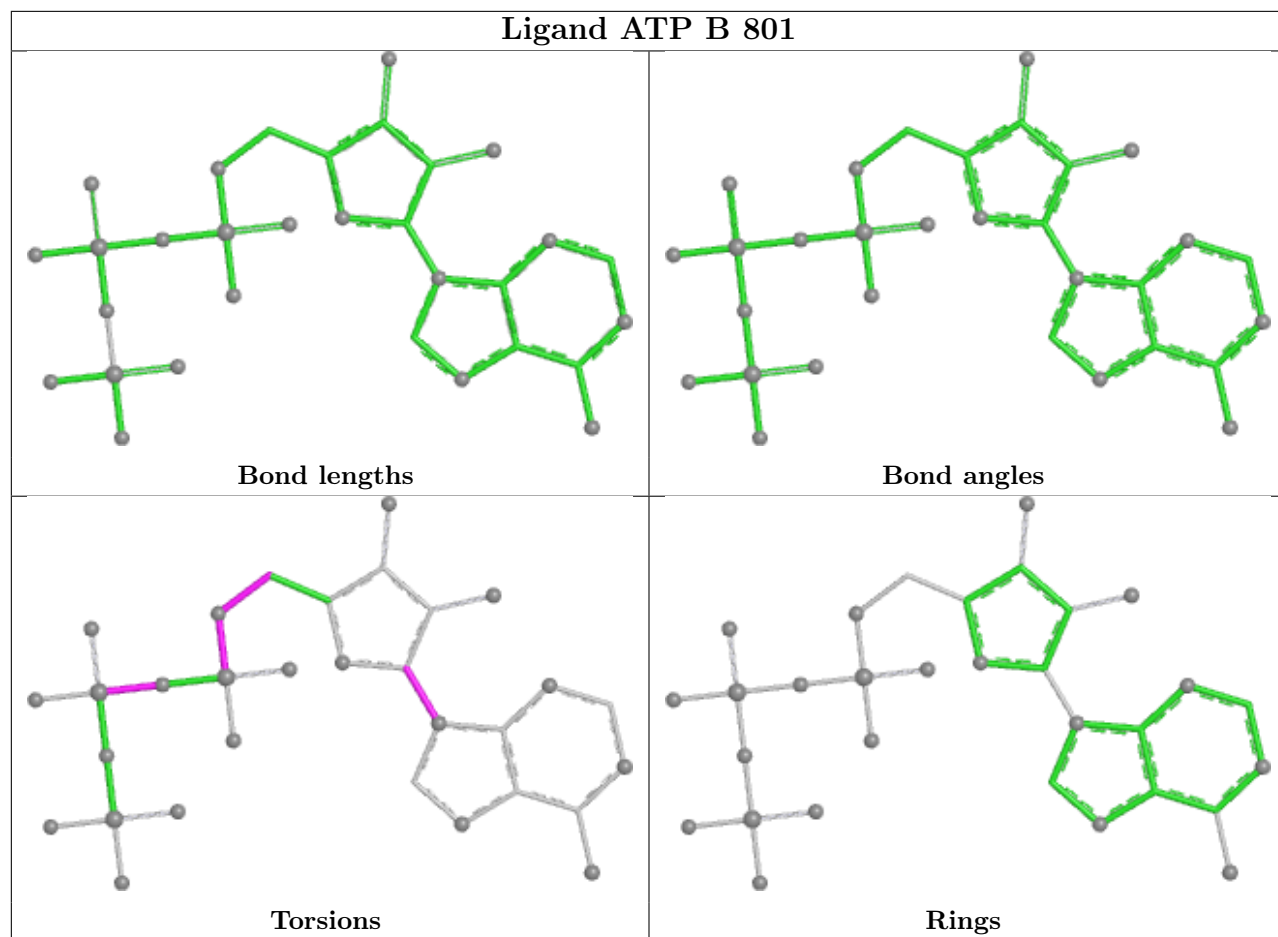
There are no ring outliers.

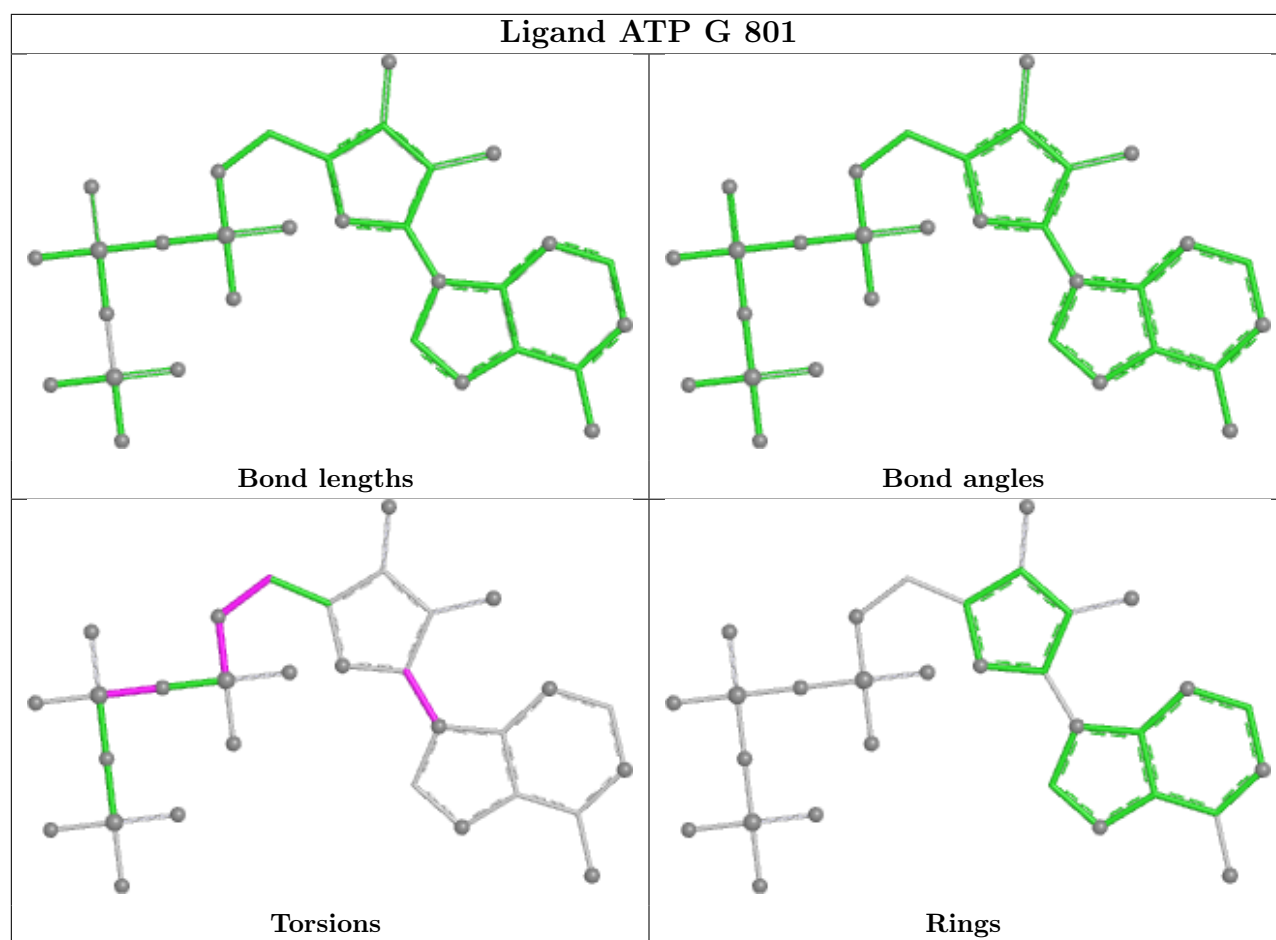
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

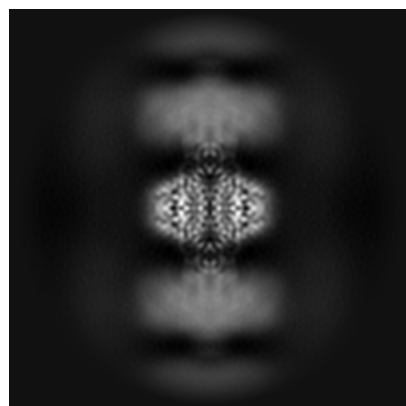
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-38855. These allow visual inspection of the internal detail of the map and identification of artifacts.

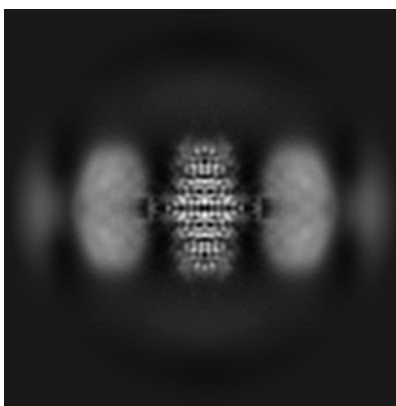
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

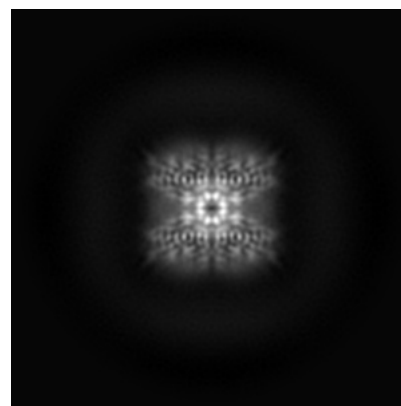
6.1.1 Primary map



X

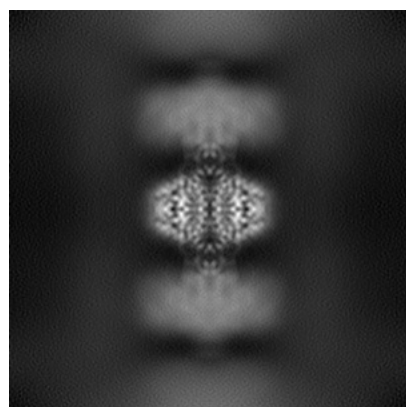


Y

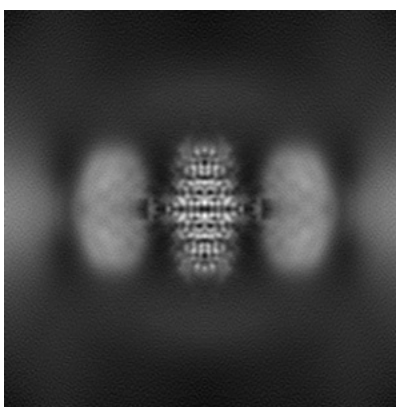


Z

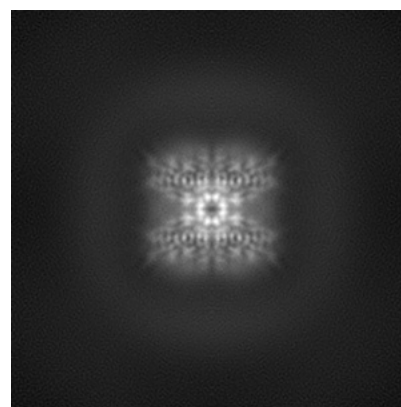
6.1.2 Raw map



X



Y

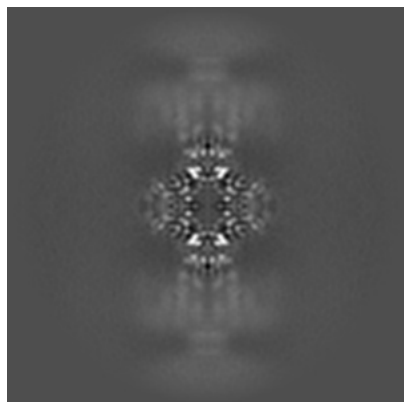


Z

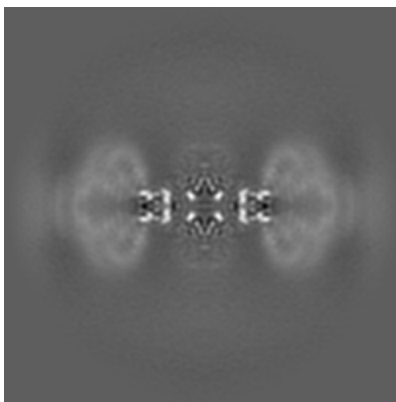
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

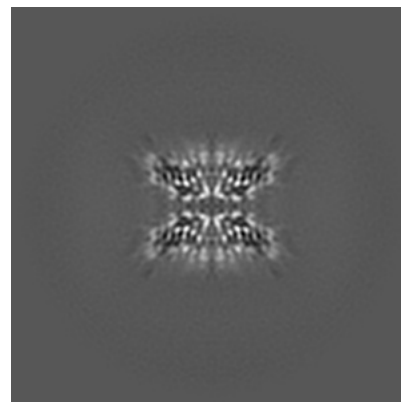
6.2.1 Primary map



X Index: 120

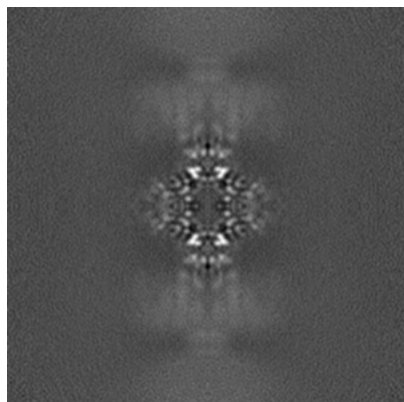


Y Index: 120

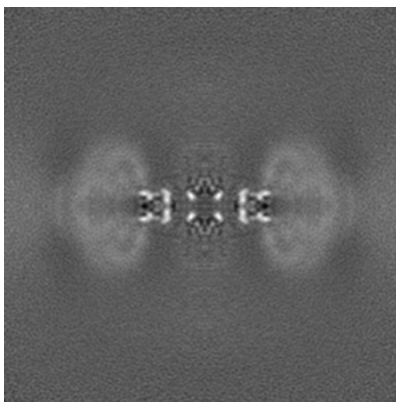


Z Index: 120

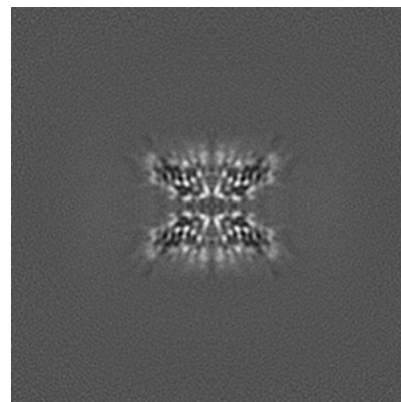
6.2.2 Raw map



X Index: 120



Y Index: 120

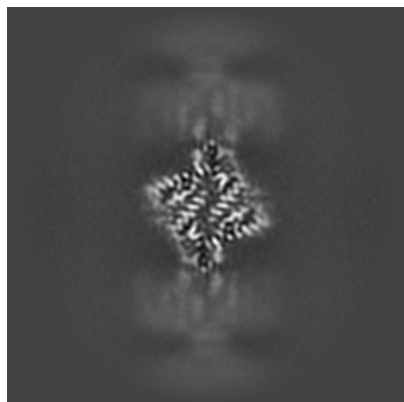


Z Index: 120

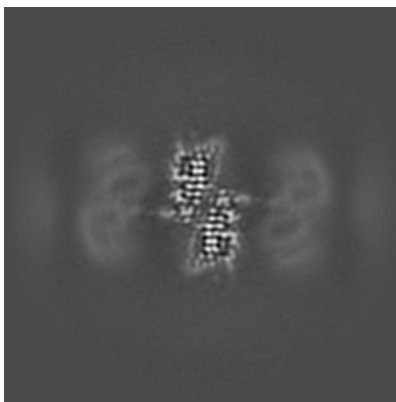
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

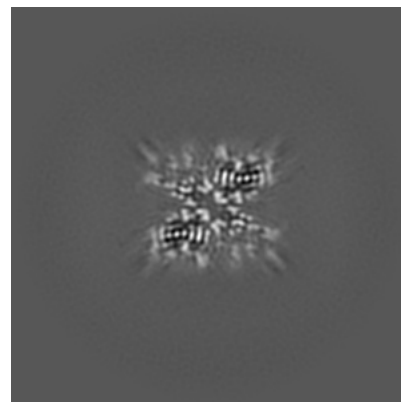
6.3.1 Primary map



X Index: 117

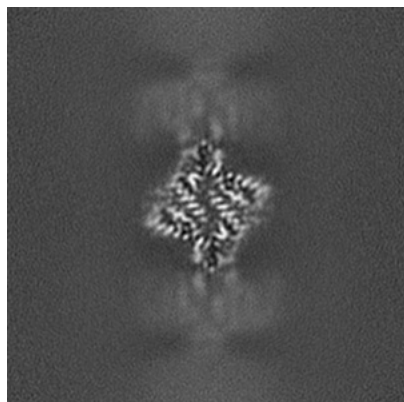


Y Index: 103

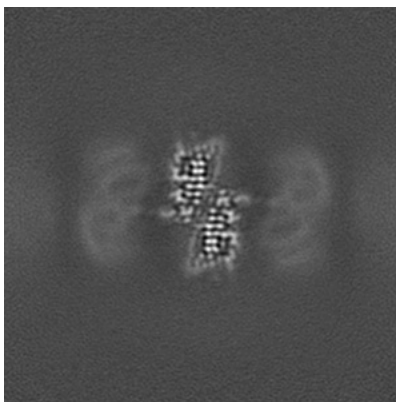


Z Index: 124

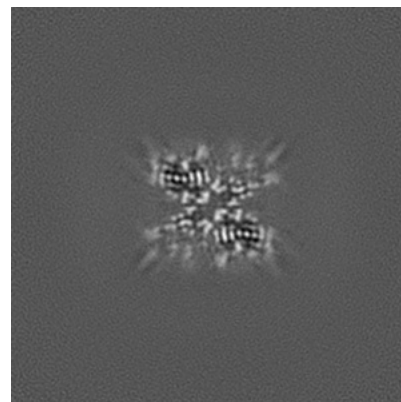
6.3.2 Raw map



X Index: 123



Y Index: 103

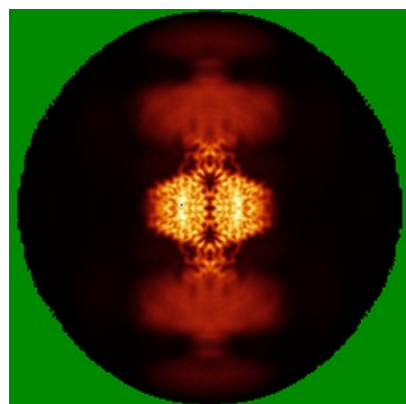


Z Index: 116

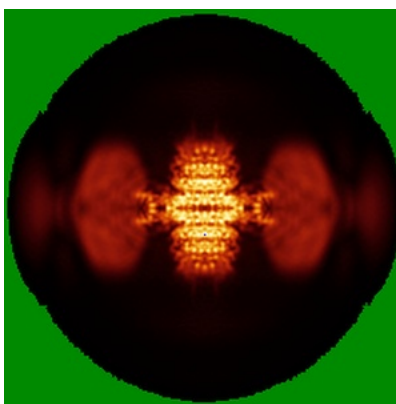
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) ⓘ

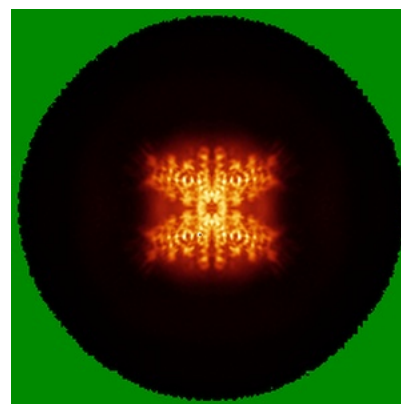
6.4.1 Primary map



X

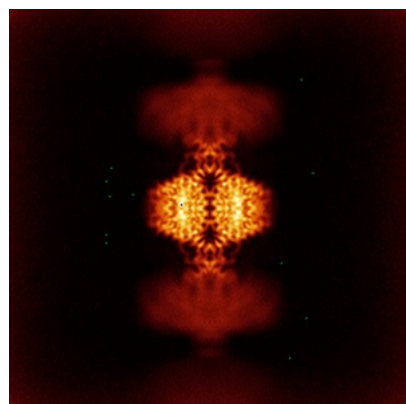


Y

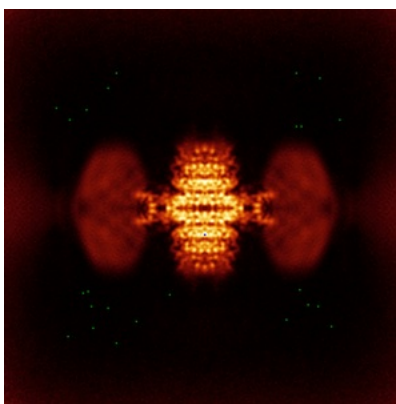


Z

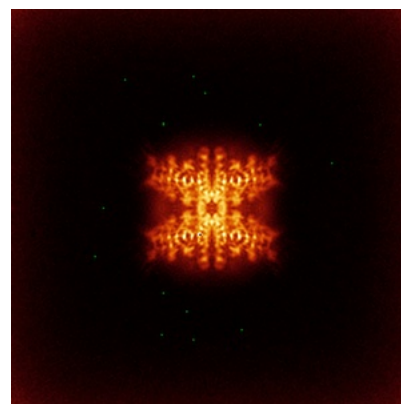
6.4.2 Raw map



X



Y



Z

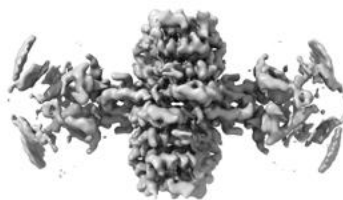
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

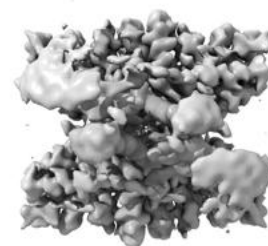
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

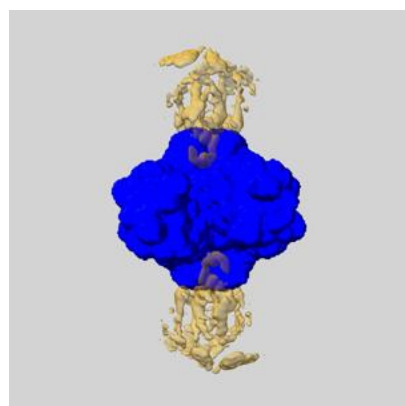
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

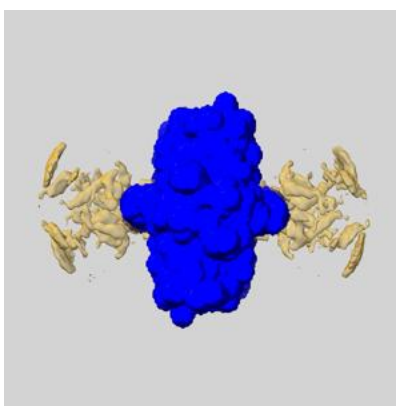
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

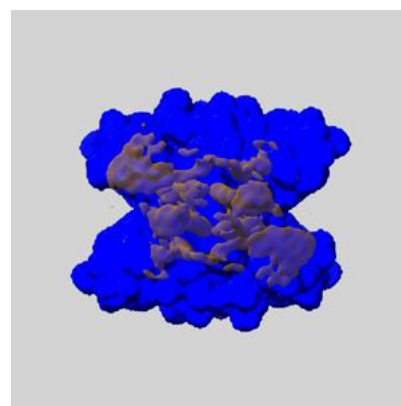
6.6.1 emd_38855_msk_1.map [i](#)



X



Y

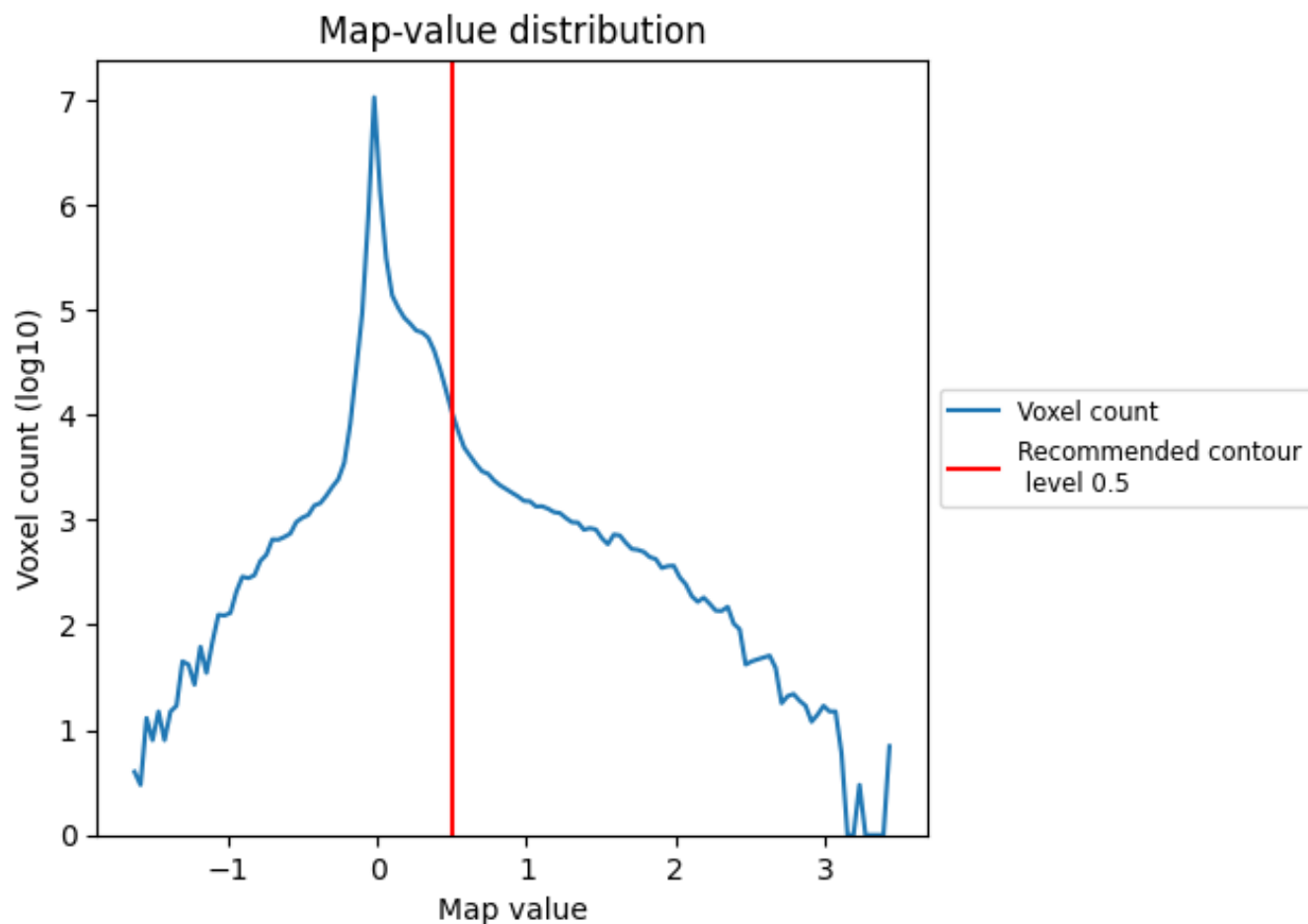


Z

7 Map analysis [i](#)

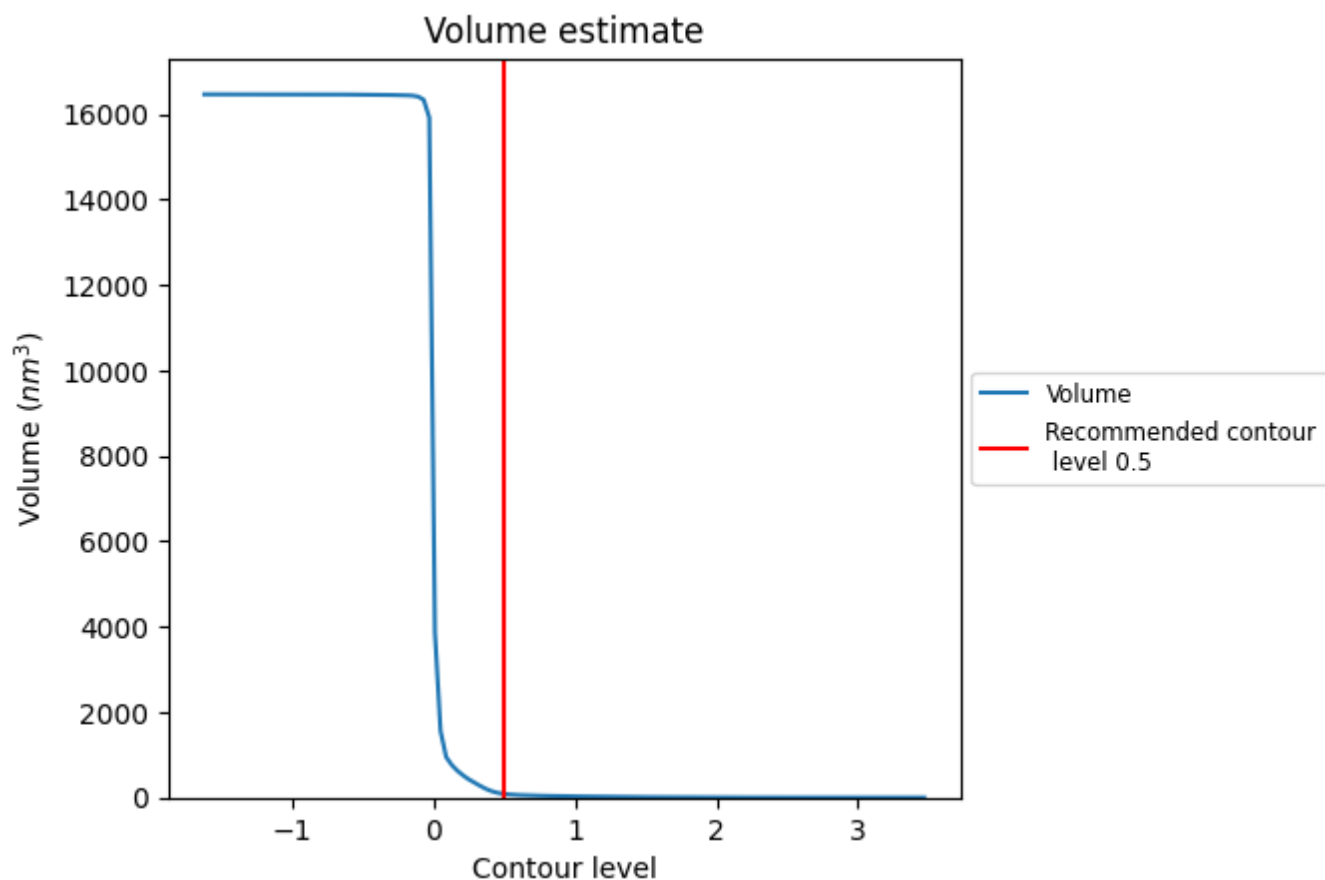
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

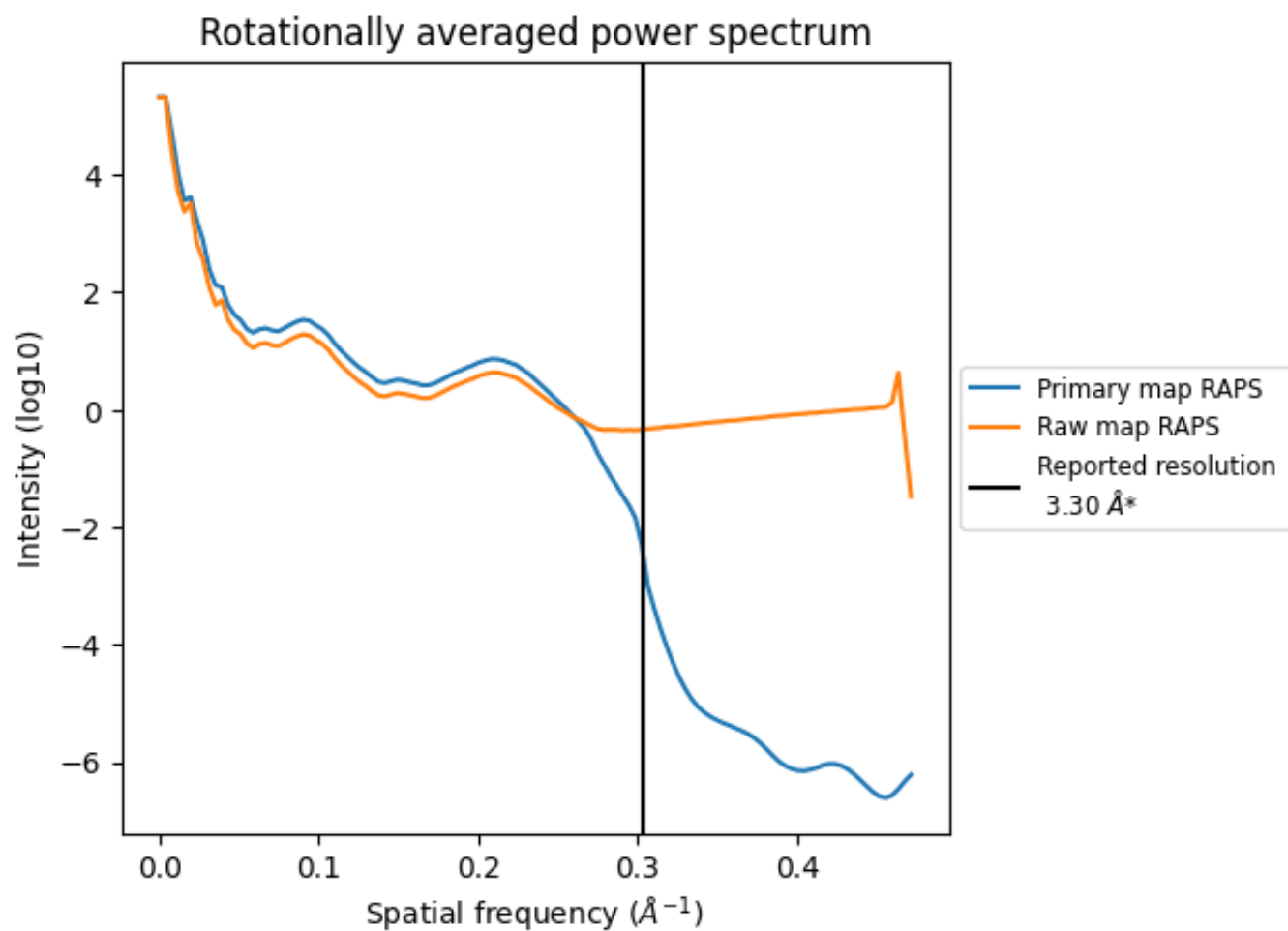
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 84 nm^3 ; this corresponds to an approximate mass of 76 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

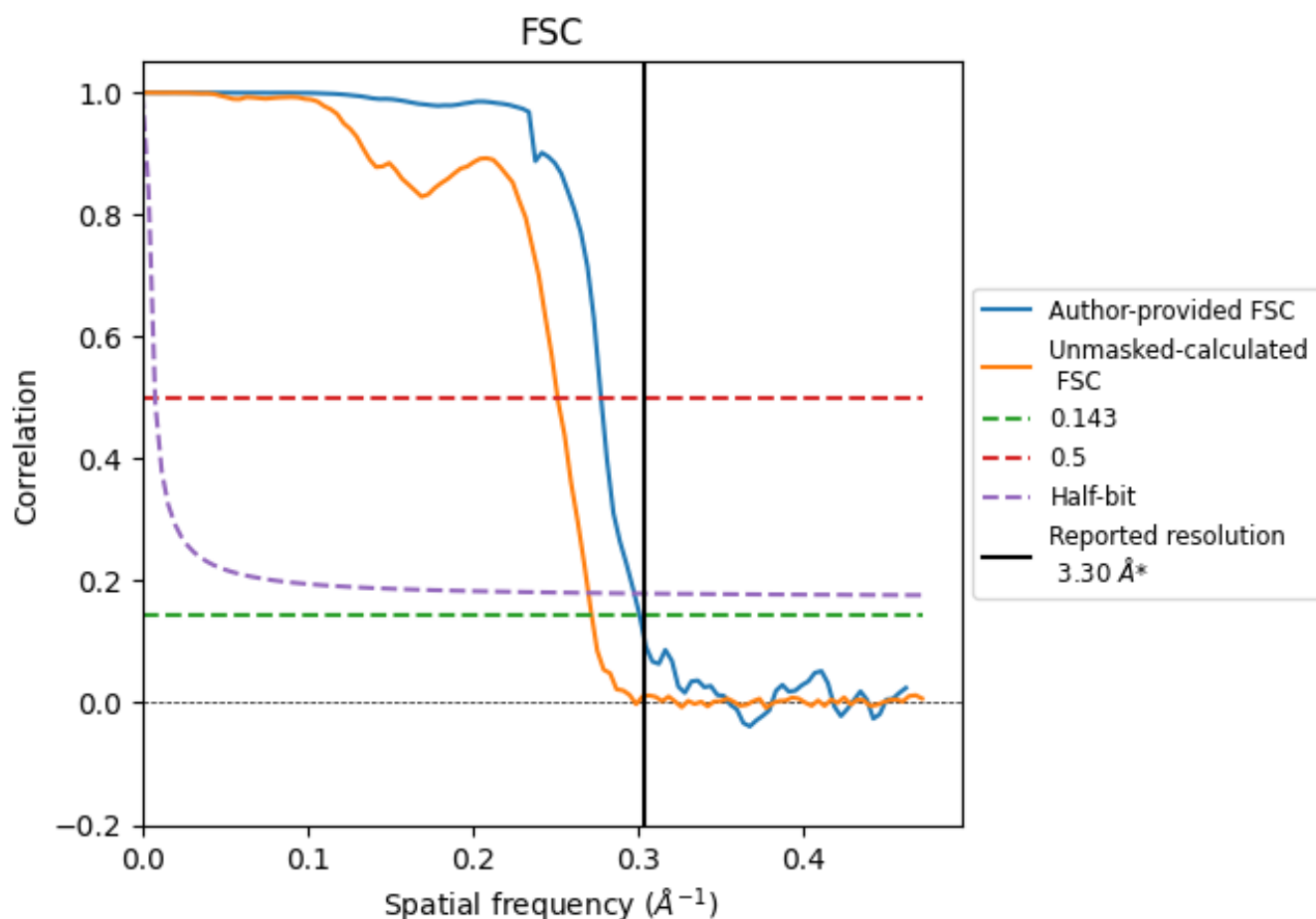


*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.32	3.60	3.36
Unmasked-calculated*	3.68	3.98	3.71

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.68 differs from the reported value 3.3 by more than 10 %

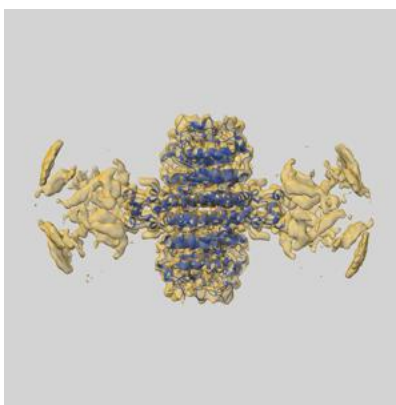
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-38855 and PDB model 8Y2H. Per-residue inclusion information can be found in section [3](#) on page [8](#).

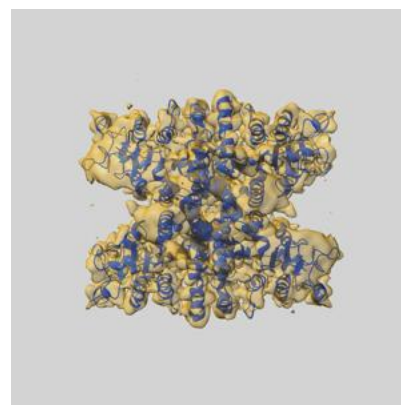
9.1 Map-model overlay [i](#)



X



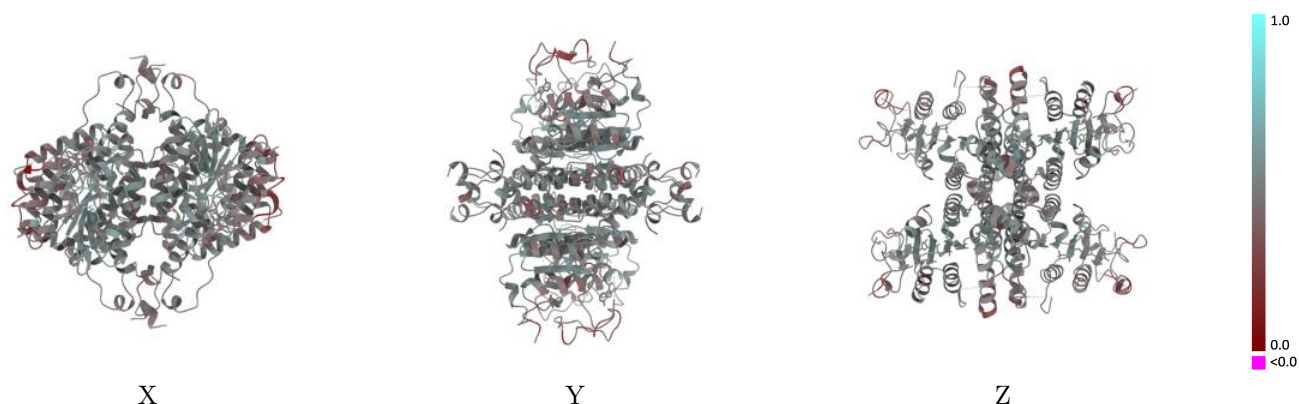
Y



Z

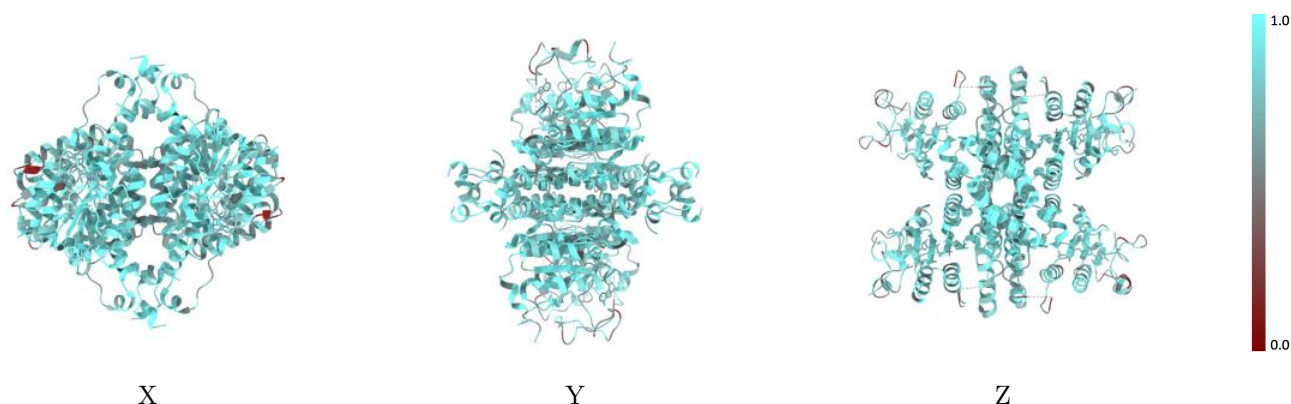
The images above show the 3D surface view of the map at the recommended contour level 0.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



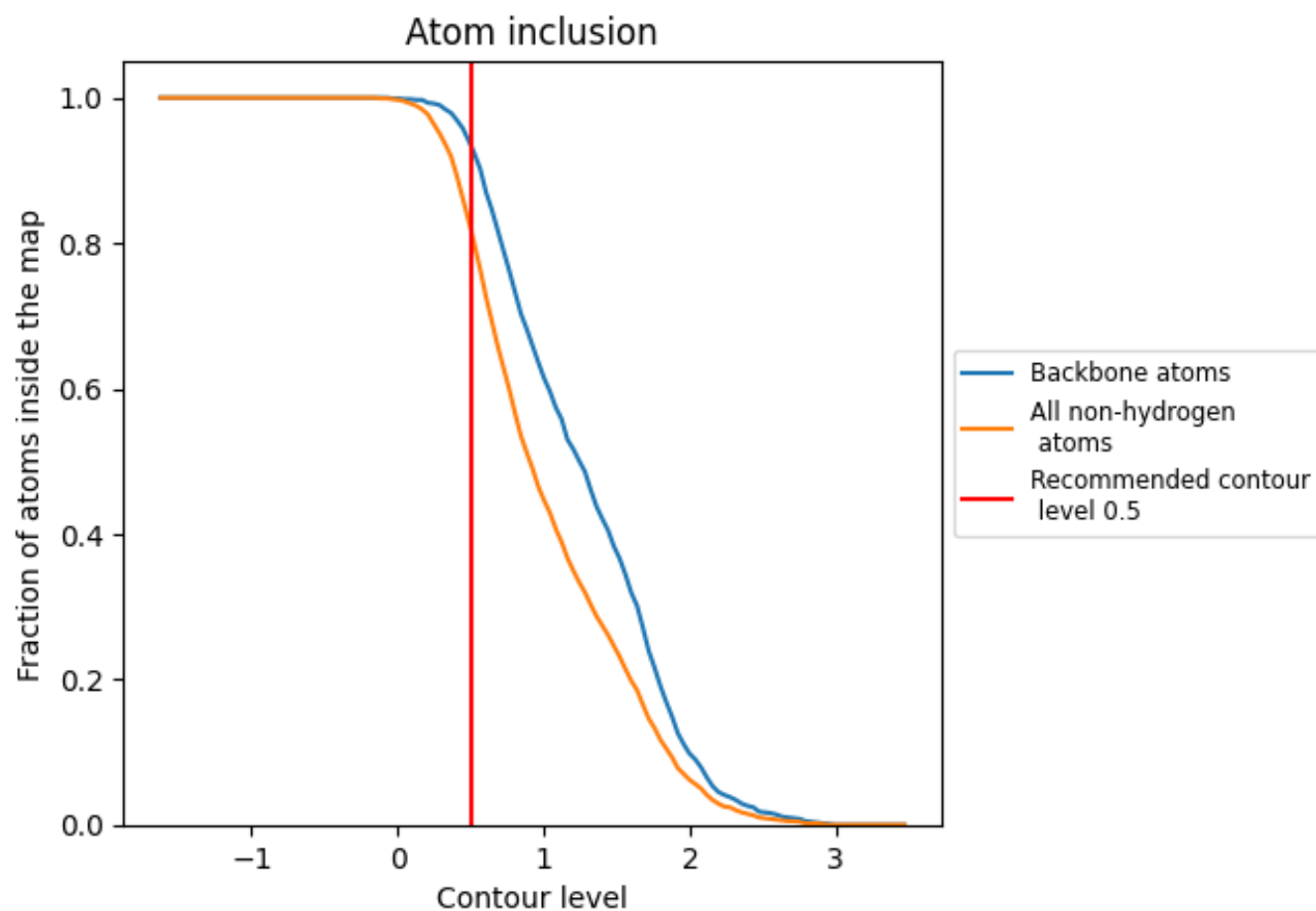
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.5).

9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 82% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8200	0.4710
A	0.8760	0.4410
B	0.8160	0.4730
C	0.8680	0.4420
D	0.8680	0.4440
E	0.8680	0.4410
F	0.8190	0.4740
G	0.8150	0.4710
H	0.8170	0.4740

